Glutaric acid, cyclohexylmethyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C19H25FO5/c1-23-17-12-15(20)10-11-16(17)25-19(22)9-5-8-18(21)24-13-14-6

InchiKey: VGPWCRAGGVVONT-UHFFFAOYSA-N

Formula: C19H25FO5

SMILES: COc1cc(F)ccc1OC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 352.40

Physical Properties

Property code	Value	Unit	Source
gf	-540.95	kJ/mol	Joback Method
hf	-985.51	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	81.82	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.034		Crippen Method
mcvol	266.470	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	2525.00		NIST Webbook
tb	864.58	K	Joback Method
tc	1079.33	K	Joback Method
tf	529.87	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.43	J/mol×K	864.58	Joback Method
cpg	864.99	J/mol×K	900.37	Joback Method
cpg	879.09	J/mol×K	936.16	Joback Method
cpg	891.74	J/mol×K	971.96	Joback Method
cpg	902.94	J/mol×K	1007.75	Joback Method
cpg	912.69	J/mol×K	1043.54	Joback Method
cpg	921.00	J/mol×K	1079.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume